Optimized statistical ensembles

for slowly equilibrating classical and quantum systems

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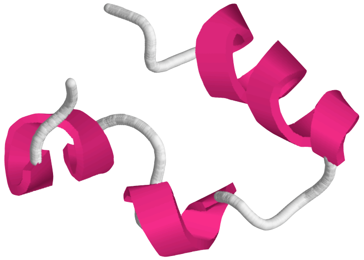
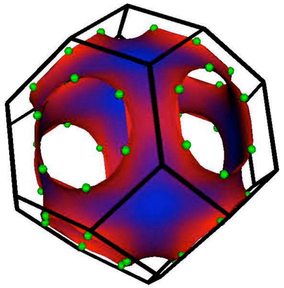
Motivation

Many interesting phenomena in complex many-body systems arise only in the presence of

- **multiple energy scales**
- **strong coupling**
- **complex energy landscapes**
- **slow equilibration**

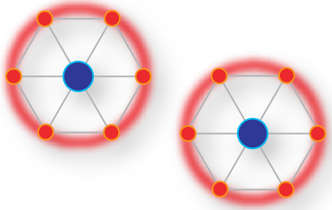

critical behavior


folding of proteins


frustrated magnets

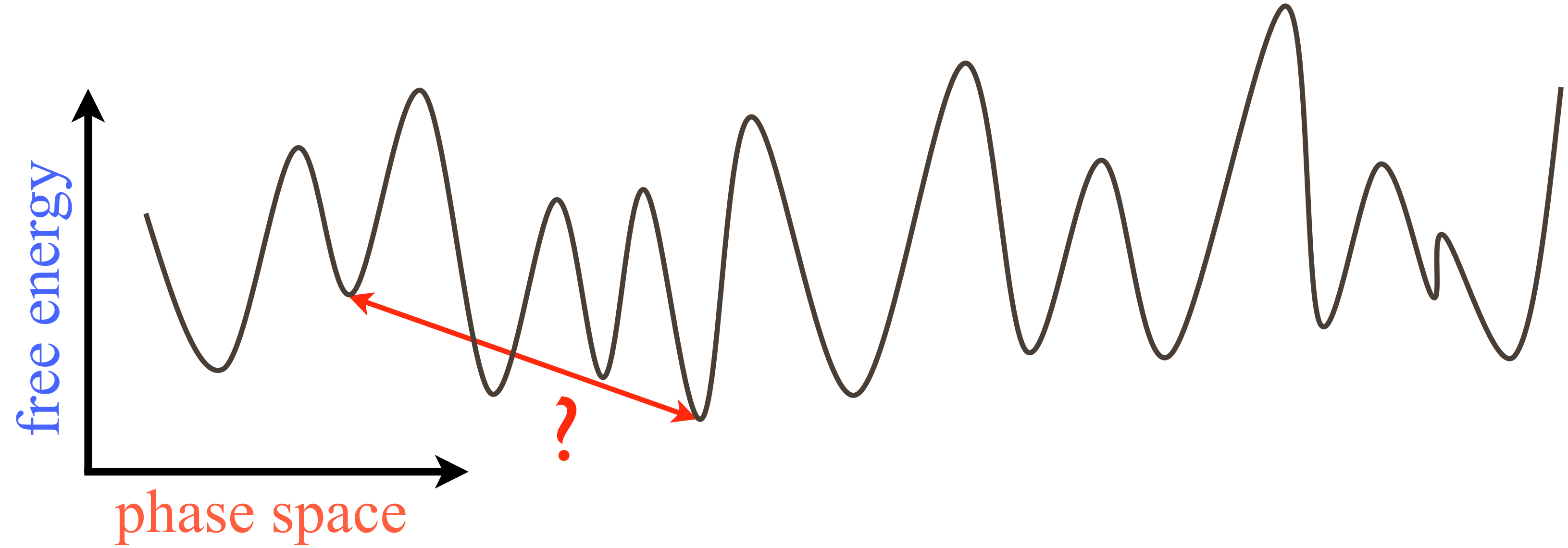
quantum systems

$\hbar$


dense liquids

Complex energy landscapes

Complex energy landscapes are characterized by **many local minima**.



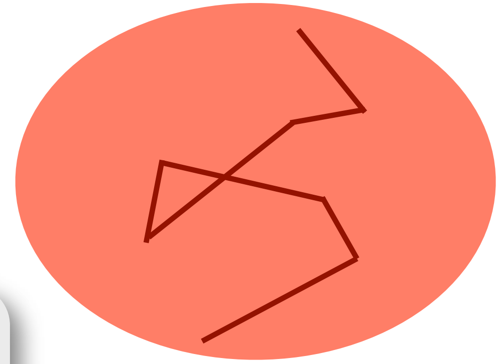
Slow equilibration due to suppressed tunneling.

How can we efficiently simulate such systems?

Simulation of Markov chains

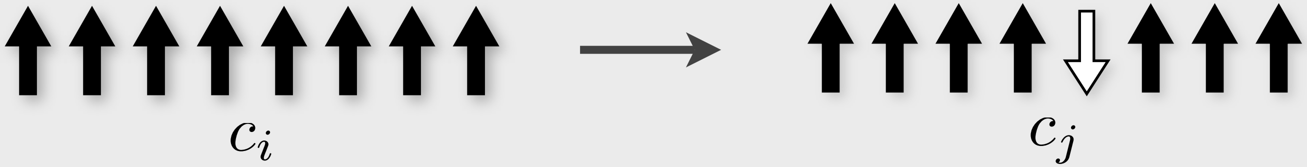
- Sample configurations in **phase space**

$$c_1 \longrightarrow c_2 \longrightarrow \ldots \longrightarrow c_i \longrightarrow c_{i+1} \longrightarrow \ldots$$



Metropolis algorithm (1953)

propose a (small) change to a configuration



accept/reject the update with probability

$$p_{acc} = \min\left(1, \frac{w(c_j)}{w(c_i)}\right)$$

How do we choose the weights?

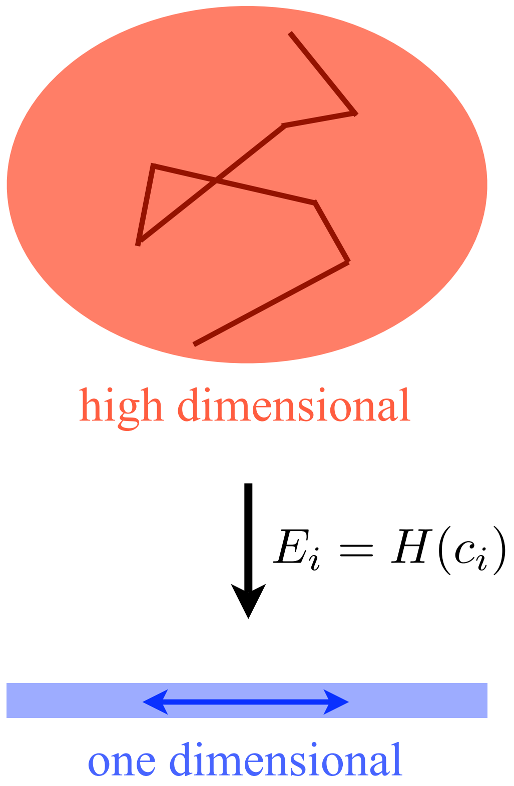
Statistical ensembles

- Sample configurations in **phase space**

$$c_1 \longrightarrow c_2 \longrightarrow \ldots \longrightarrow c_i \longrightarrow c_{i+1} \longrightarrow \ldots$$

- Project onto random walk in **energy space**

$$E_1 \longrightarrow E_2 \longrightarrow \ldots \longrightarrow E_i \longrightarrow E_{i+1} \longrightarrow \ldots$$



- We define a **statistical ensemble**

$$w(c_i) = w(E_i) = \exp(-\beta E_i)$$

$$p_{acc}(E_1 \rightarrow E_2) = \min\left(1, \frac{w(E_2)}{w(E_1)}\right) = \min\left(1, \exp(-\beta \Delta E)\right)$$

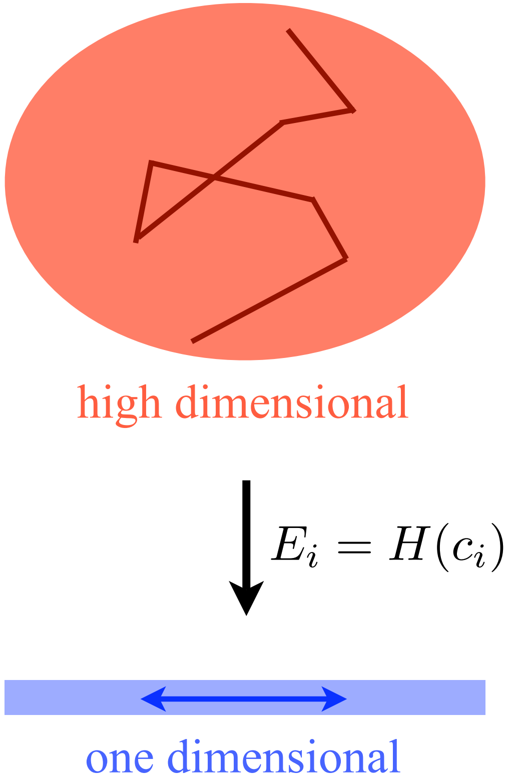
Statistical ensembles

- Sample configurations in **phase space**

$$c_1 \longrightarrow c_2 \longrightarrow \ldots \longrightarrow c_i \longrightarrow c_{i+1} \longrightarrow \ldots$$

- Project onto random walk in **energy space**

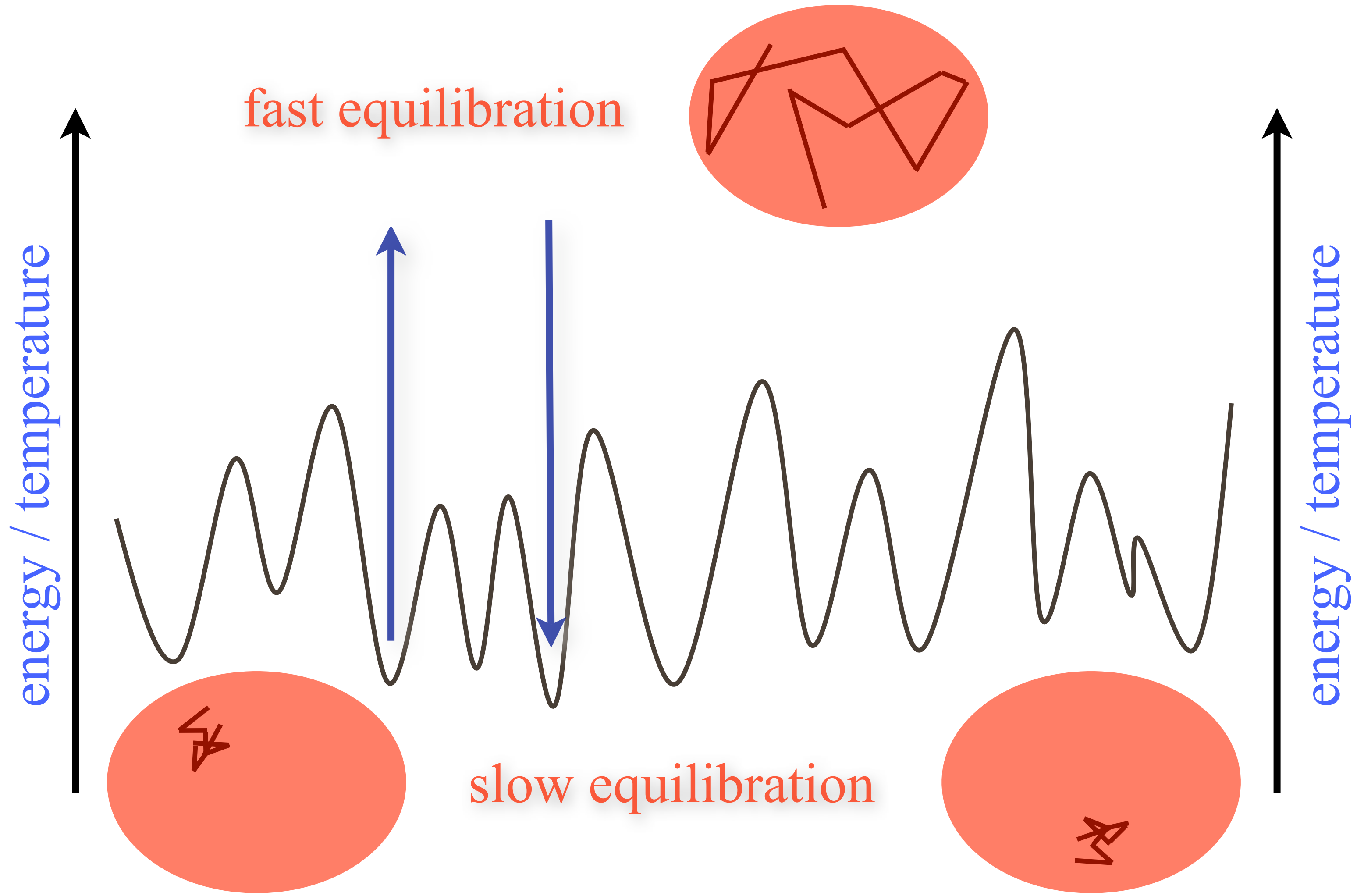
$$E_1 \longrightarrow E_2 \longrightarrow \ldots \longrightarrow E_i \longrightarrow E_{i+1} \longrightarrow \ldots$$



- **Phase space:** The simulated system does a biased and Markovian random walk.
- **Energy space:** The projected random walk is **non-Markovian**, as memory is stored in the system’s configuration.

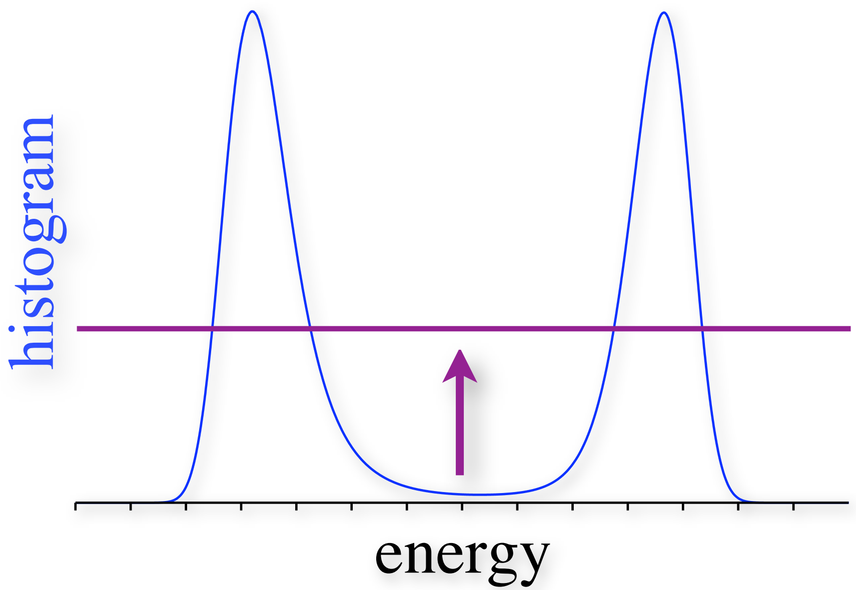
Random walks in energy

Random walk in temperature space increases equilibration.



Extended ensemble simulations

- **Broaden the sampled energy space**, e.g. by sampling a flat histogram.



$$\begin{tikzcd} w(E) = \exp(-\beta E) \arrow[d] \\ w(E) = 1/g(E) \end{tikzcd}$$

density of states

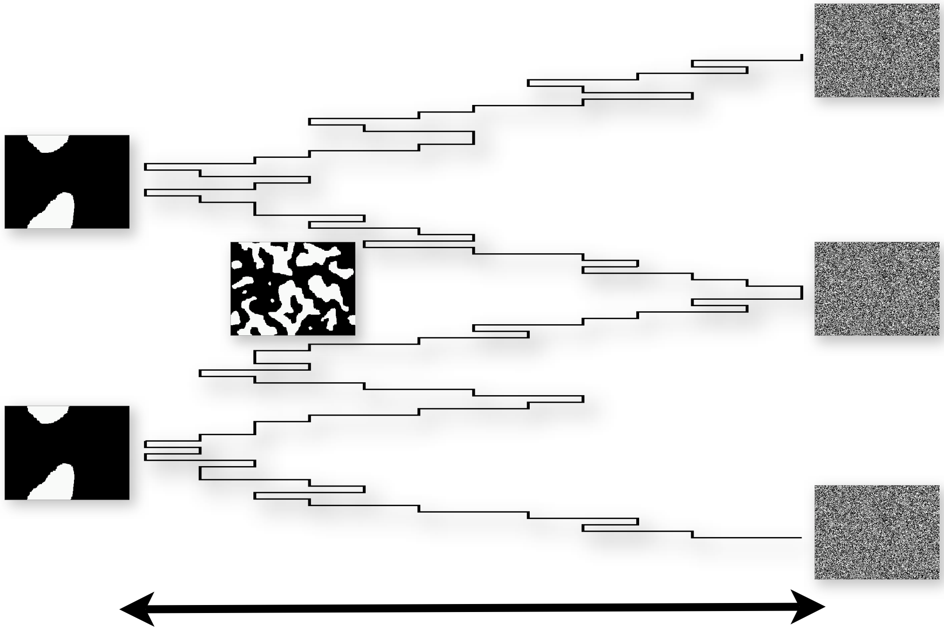
$$n_w(E) = w(E)\, g(E)$$

histogram

weight / ensemble

Wang-Landau algorithm ('01)

How well does this work?

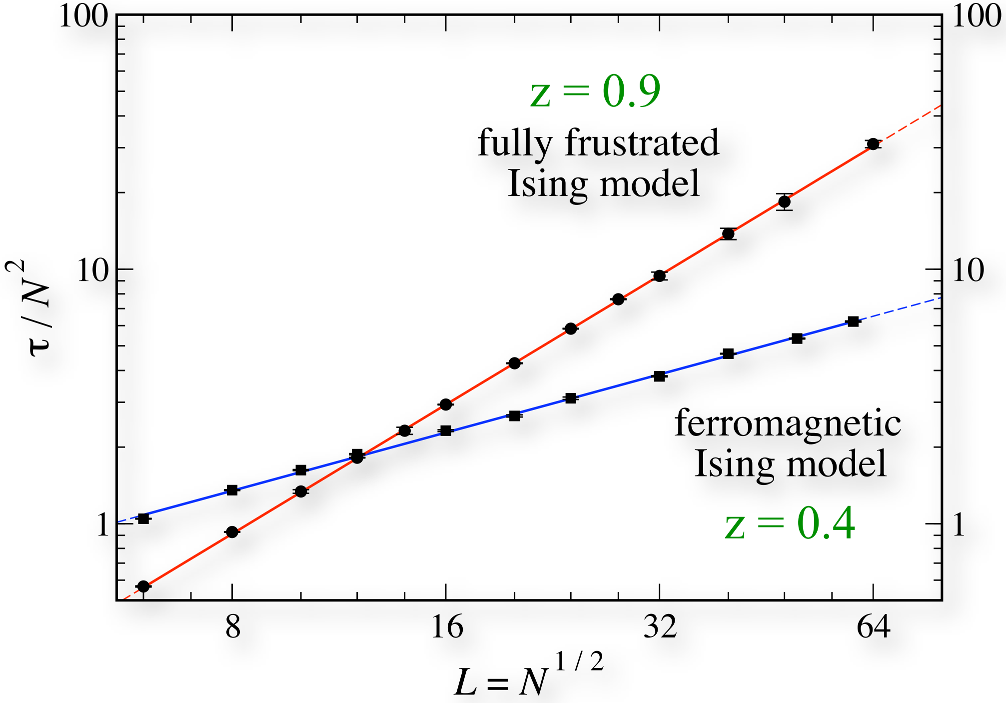


$$E \sim N$$

The energy range scales like N.

$$\tau \sim N^2$$

The round-trip time should scale like N^2.



Flat-histogram sampling

$$\tau \sim N^{2+z}$$

Critical slowing down.

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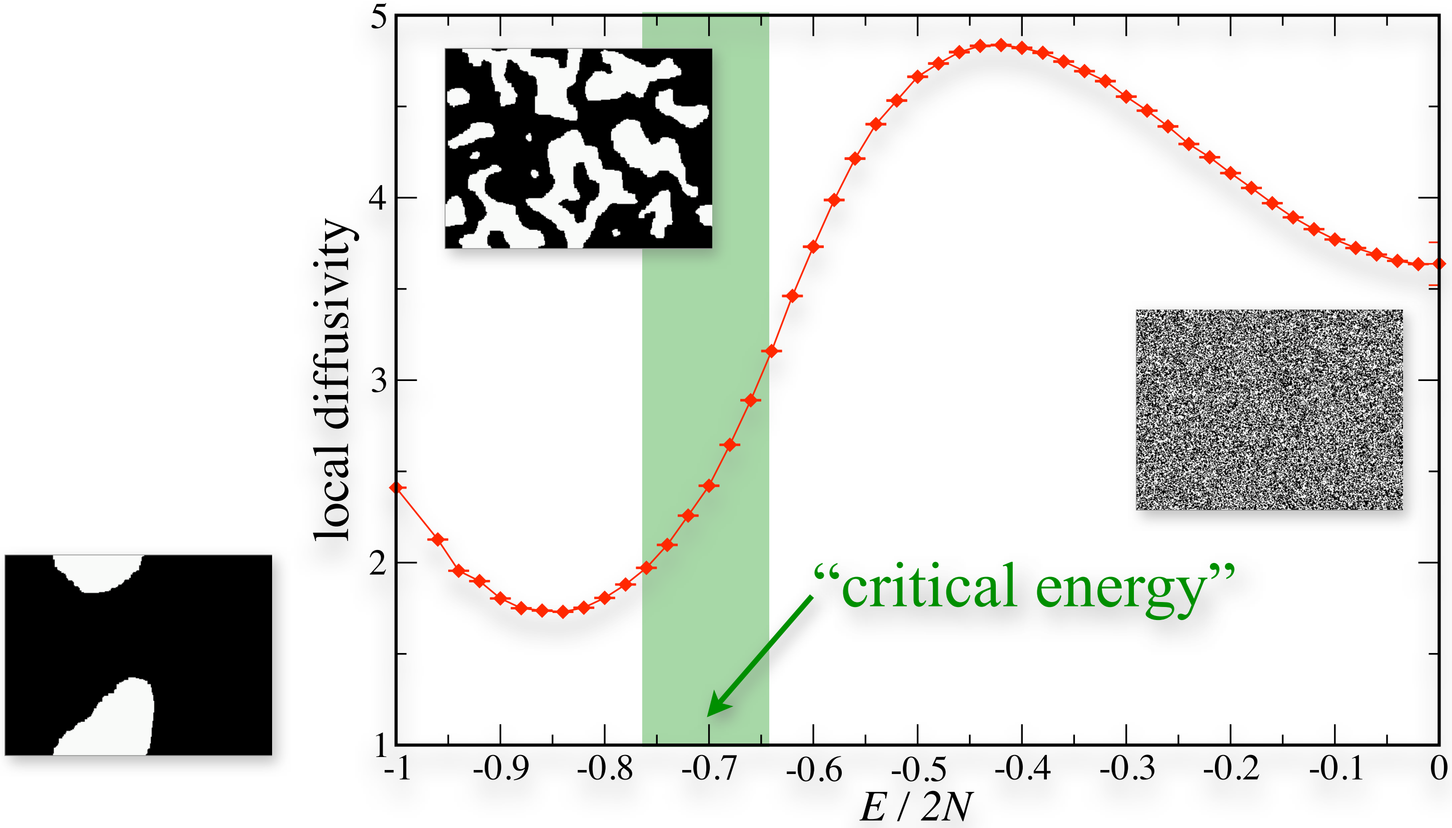
The problem: local diffusivity

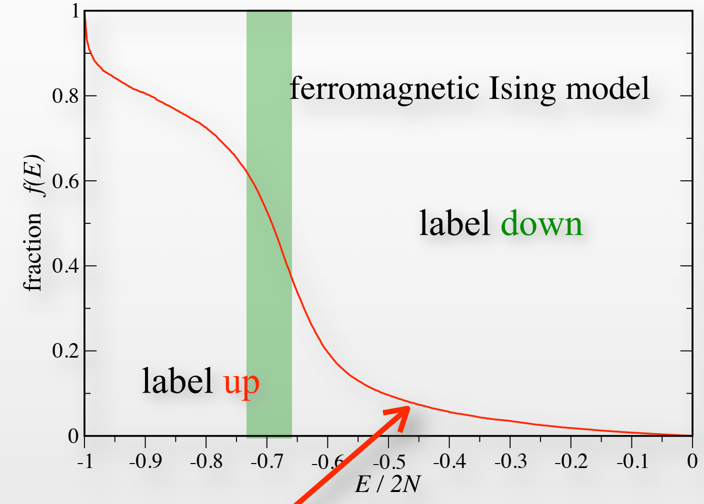
$$D(E, t_D) = \langle [E(t) - E(t + t_D)]^2 \rangle / t_D$$



- The **local diffusivity** is **NOT** independent of the energy.

Optimizing the ensemble

Measure the **current** in the energy interval



local diffusivity

$$j = D(E)\, n_w(E)\, \frac{df}{dE}$$

current

histogram

derivative of fraction

Determine the **local diffusivity**.

Maximize current by varying histogram/ensemble.

Phys. Rev. E **70**, 046701 (2004).

Optimizing the ensemble (cont'd)

Optimal histogram turns out to be

$$n_w^{(opt)}(E) \propto \frac{1}{\sqrt{D(E)}}$$

Ensemble optimization algorithm

Feedback the local diffusivity

optimized ensemble

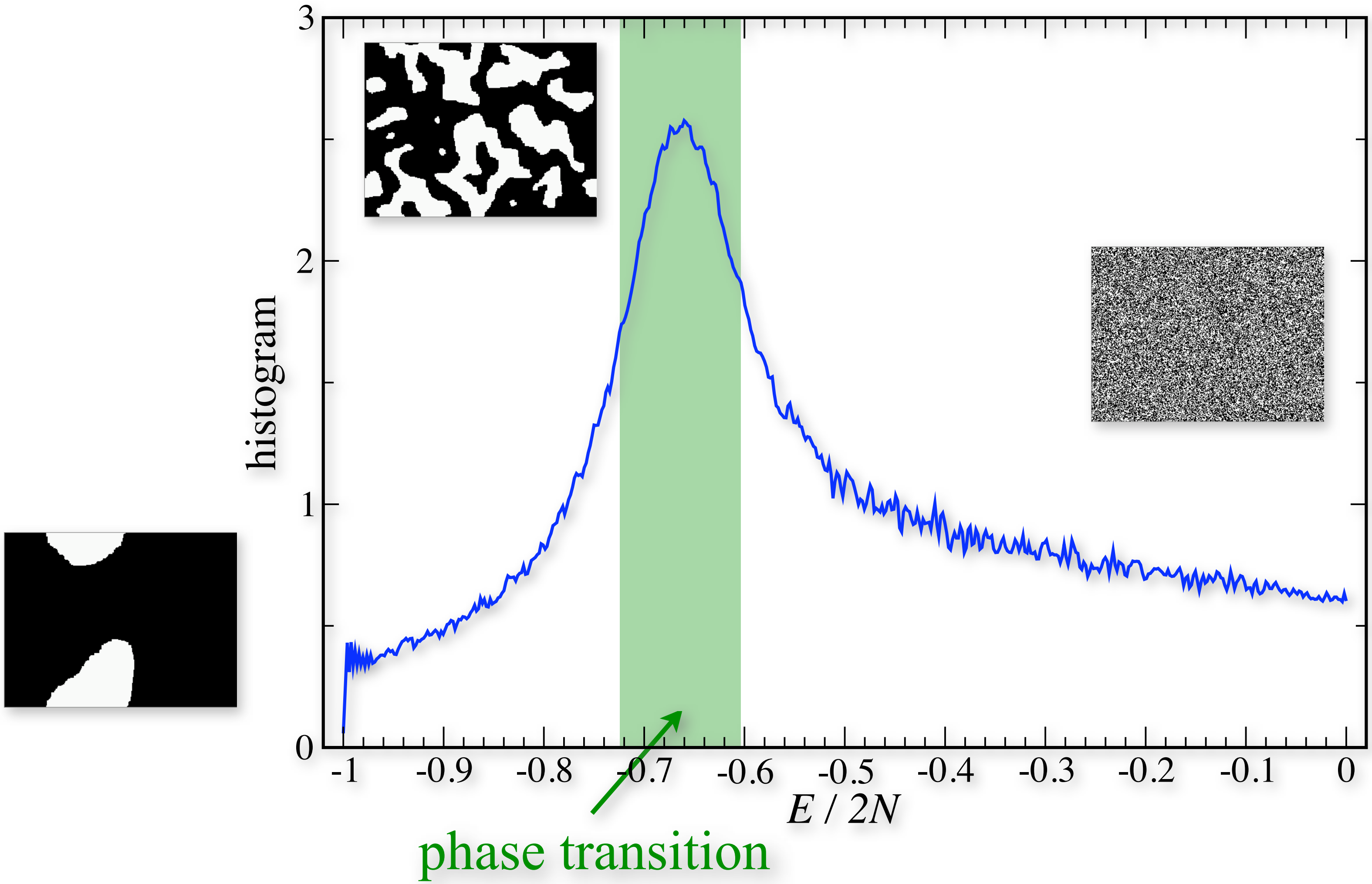
$$w'(E) \propto w(E) \cdot \sqrt{\frac{df}{dE} \cdot \frac{1}{n_w(E)}}$$

original ensemble

and **iterate** feedback until convergence.

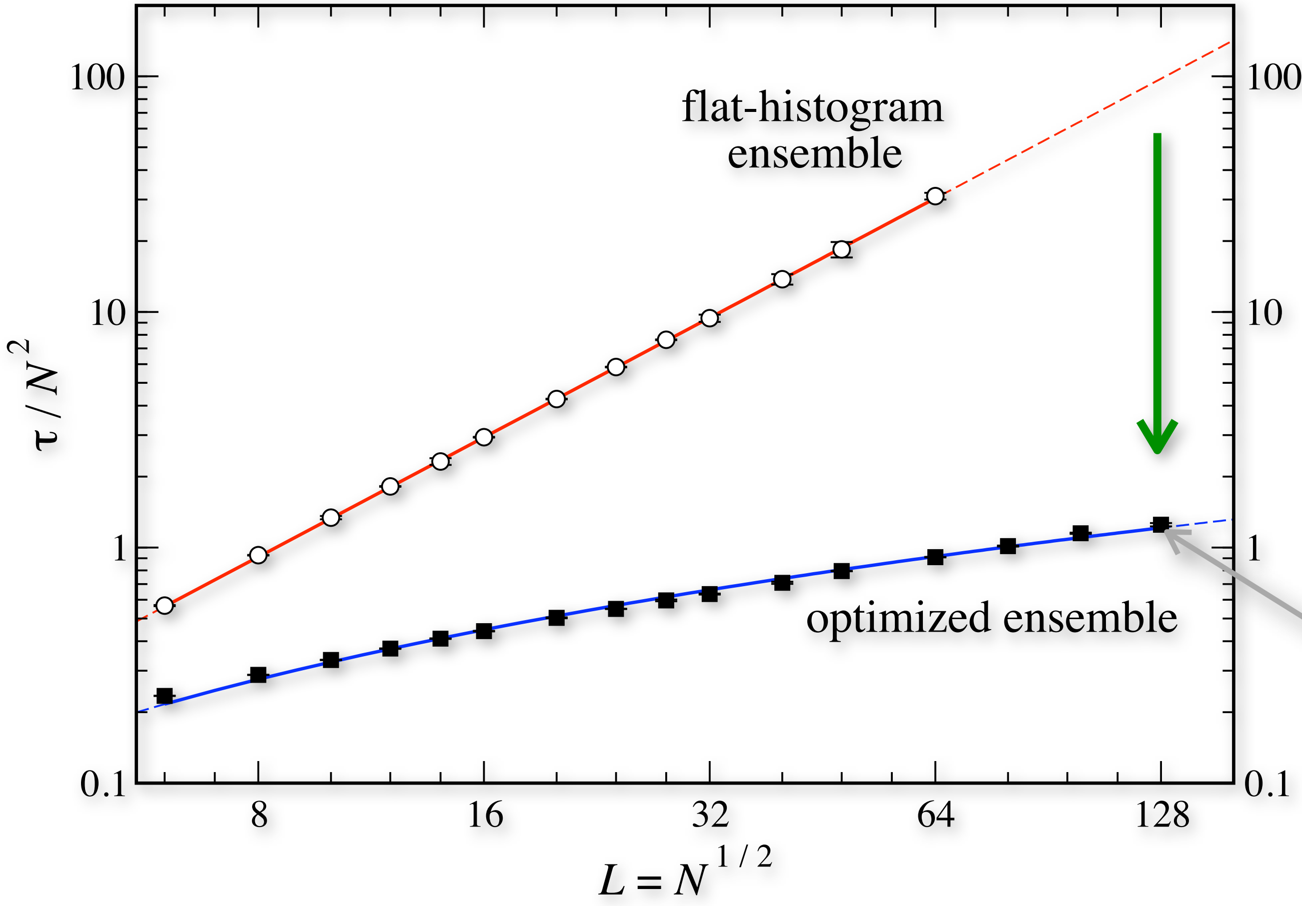
Phys. Rev. E **70**, 046701 (2004).

Optimized histogram



- **Feedback reallocates resources** towards the critical energy.

Performance of optimized ensemble



speedup ~ 100

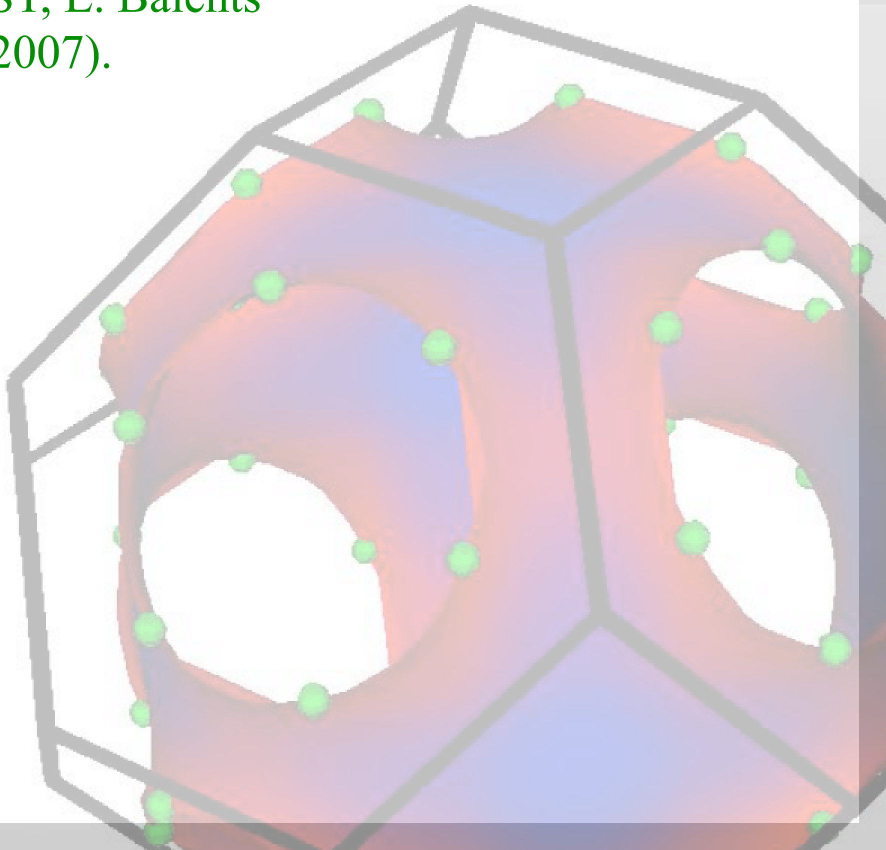
5,000 cpu hours

The round-trip times scale like $O\left([N \log N]^2\right)$.

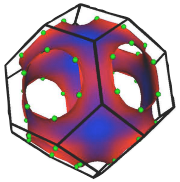
Example

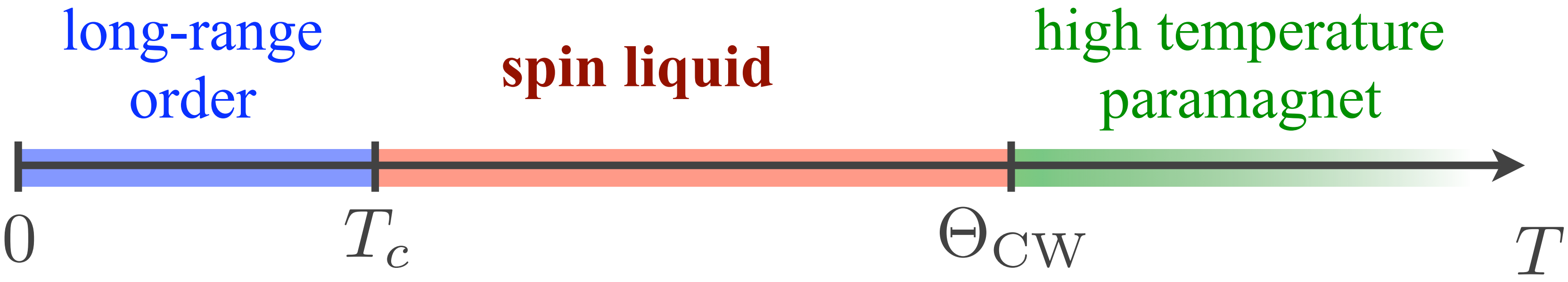
Order by disorder transitions & spiral spin liquids

D. Bergman, J. Alicea, E. Gull, ST, L. Balents
Nature Physics **3**, 487 (2007).



Frustrated magnets





frustration parameter

$$f = \frac{\Theta_{\text{CW}}}{T_c}$$

"highly frustrated"

$$f > 5 - 10$$

spin liquid

system **fluctuates** amongst low-energy configurations, but **no** long-range order

Curie-Weiss law

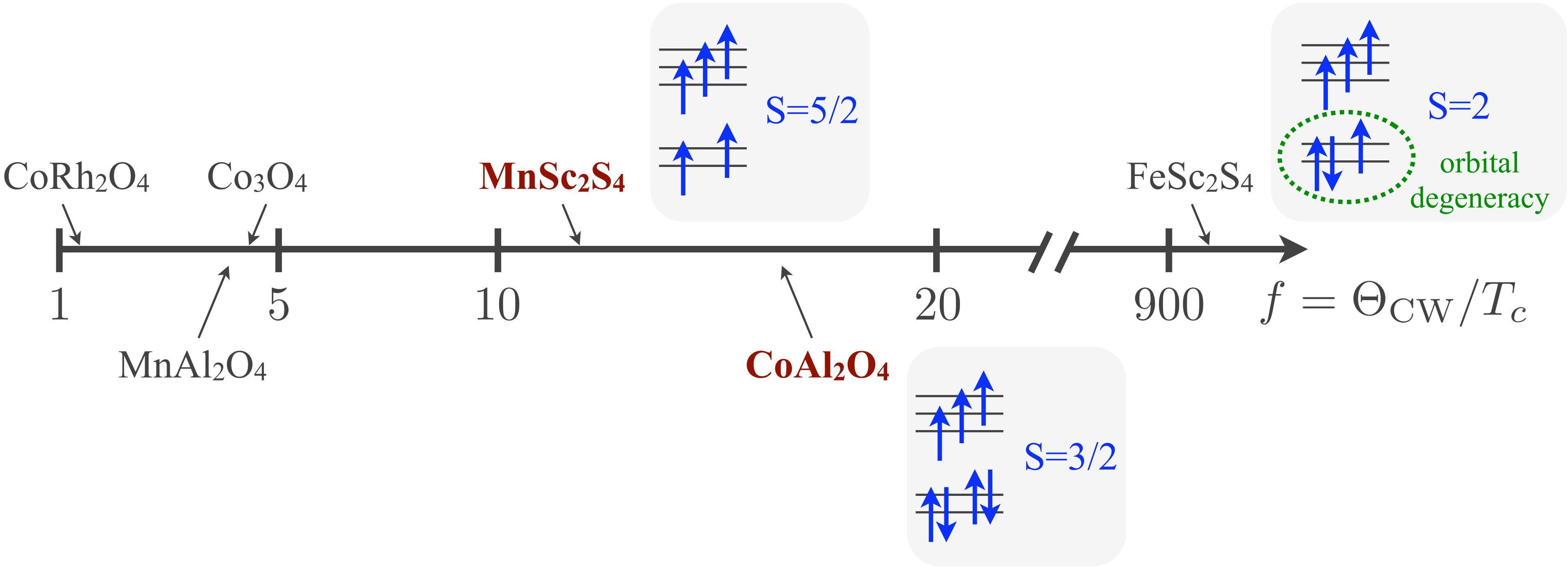
$$\chi \sim \frac{1}{T - \Theta_{\text{CW}}}$$

Diamond lattice antiferromagnets: Materials

V. Fritsch *et al.*, PRL **92**, 116401 (2004); N. Tristan *et al.*, PRB **72**, 174404 (2005); T. Suzuki *et al.* (2007)

Many materials take on the normal spinel structure AB_2X_4.

Focus: Spinels with magnetic A-sites (only).

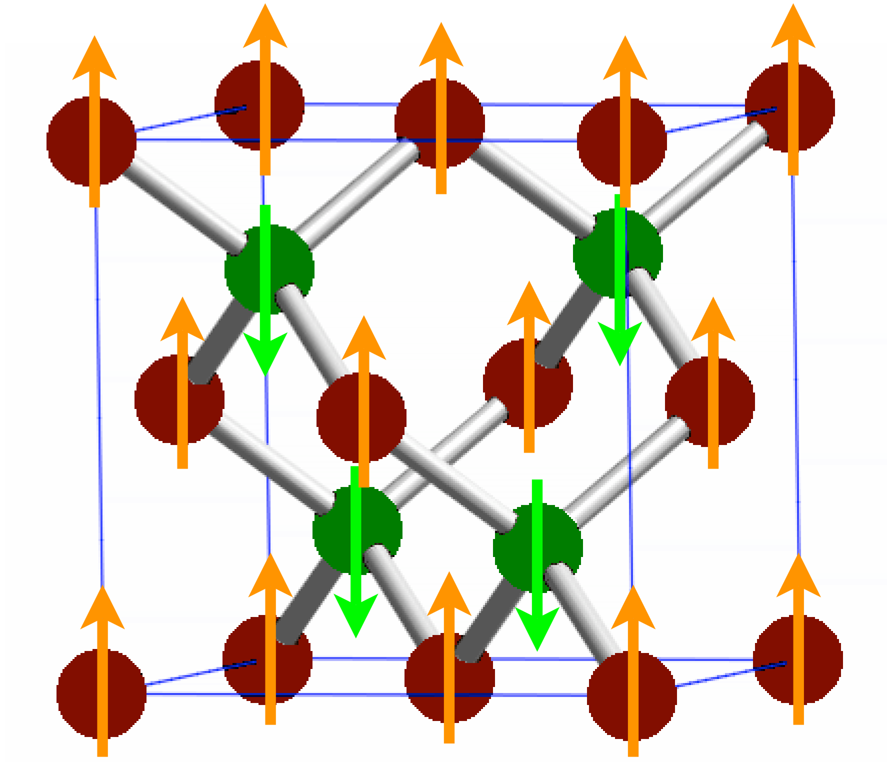


Frustration in the diamond lattice

Naive Hamiltonian $$H = \boxed{J_1} \sum_{\langle ij \rangle} \boxed{\vec{S}_i \cdot \vec{S}_j}$$

antiferromagnetic

classical spins
S=3/2, S=5/2



diamond lattice
two FCC lattices
coupled via J_1

bipartite lattice
no frustration

Frustration in the diamond lattice

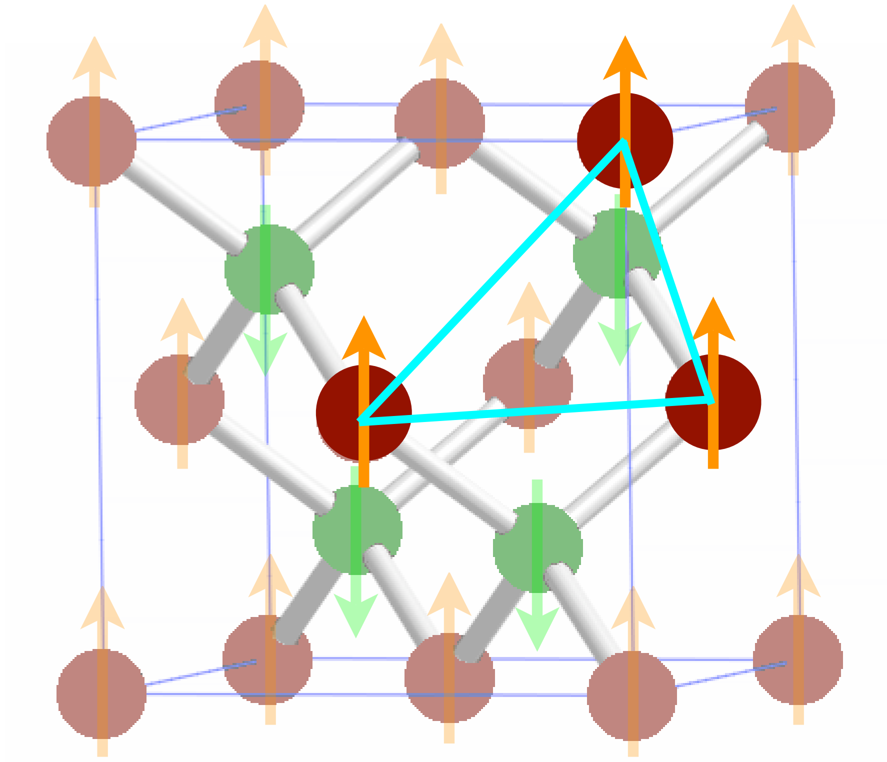
2nd neighbor exchange

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

$J_1 \approx J_2$

similar exchange path

W. L. Roth, J. Phys. **25**, 507 (1964)



J_2 generates **strong** frustration

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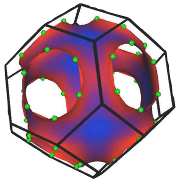
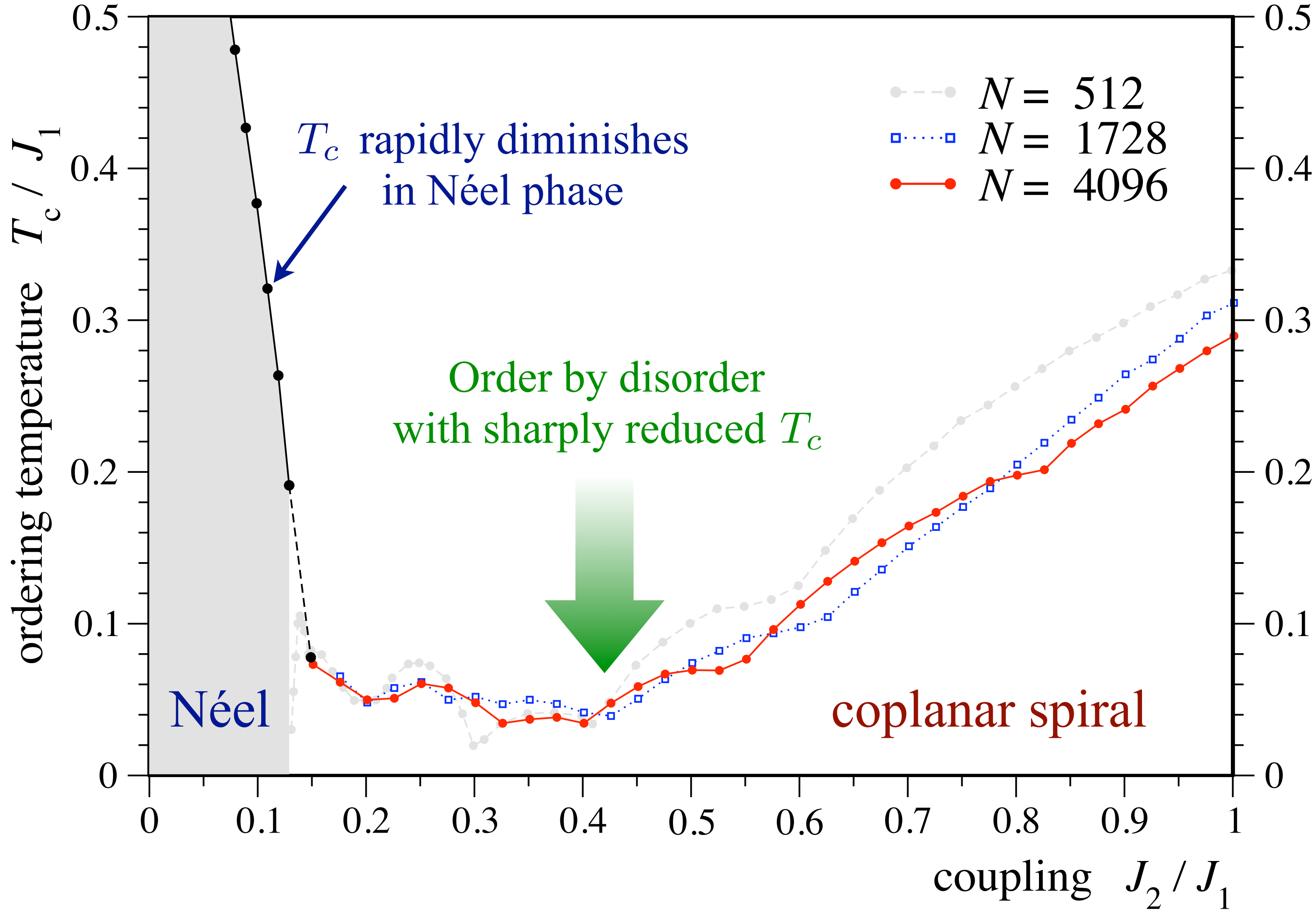
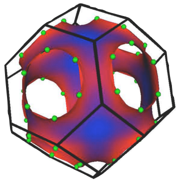
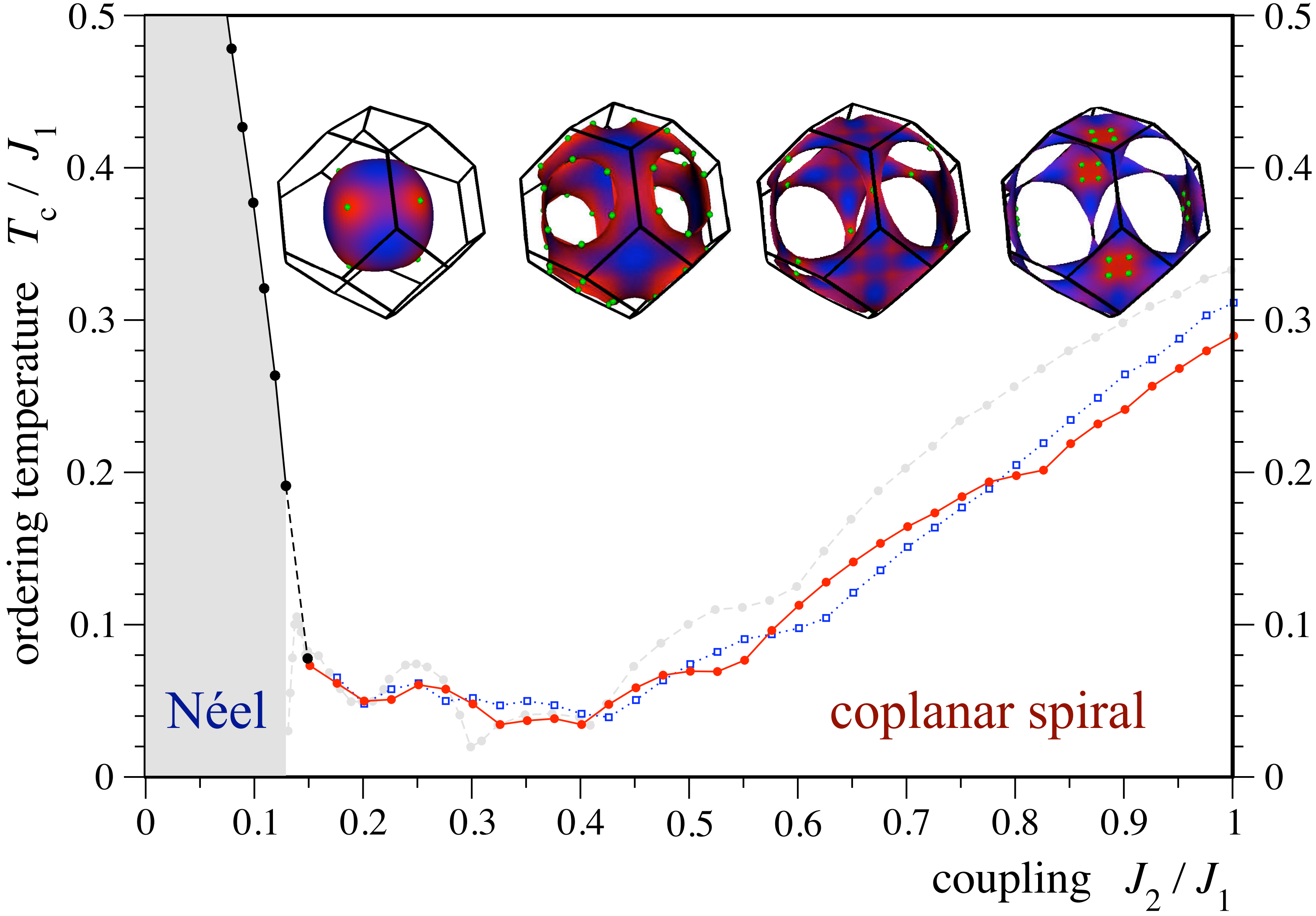
Phase diagram





Spiral surfaces





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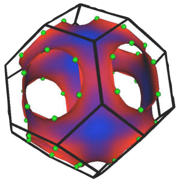
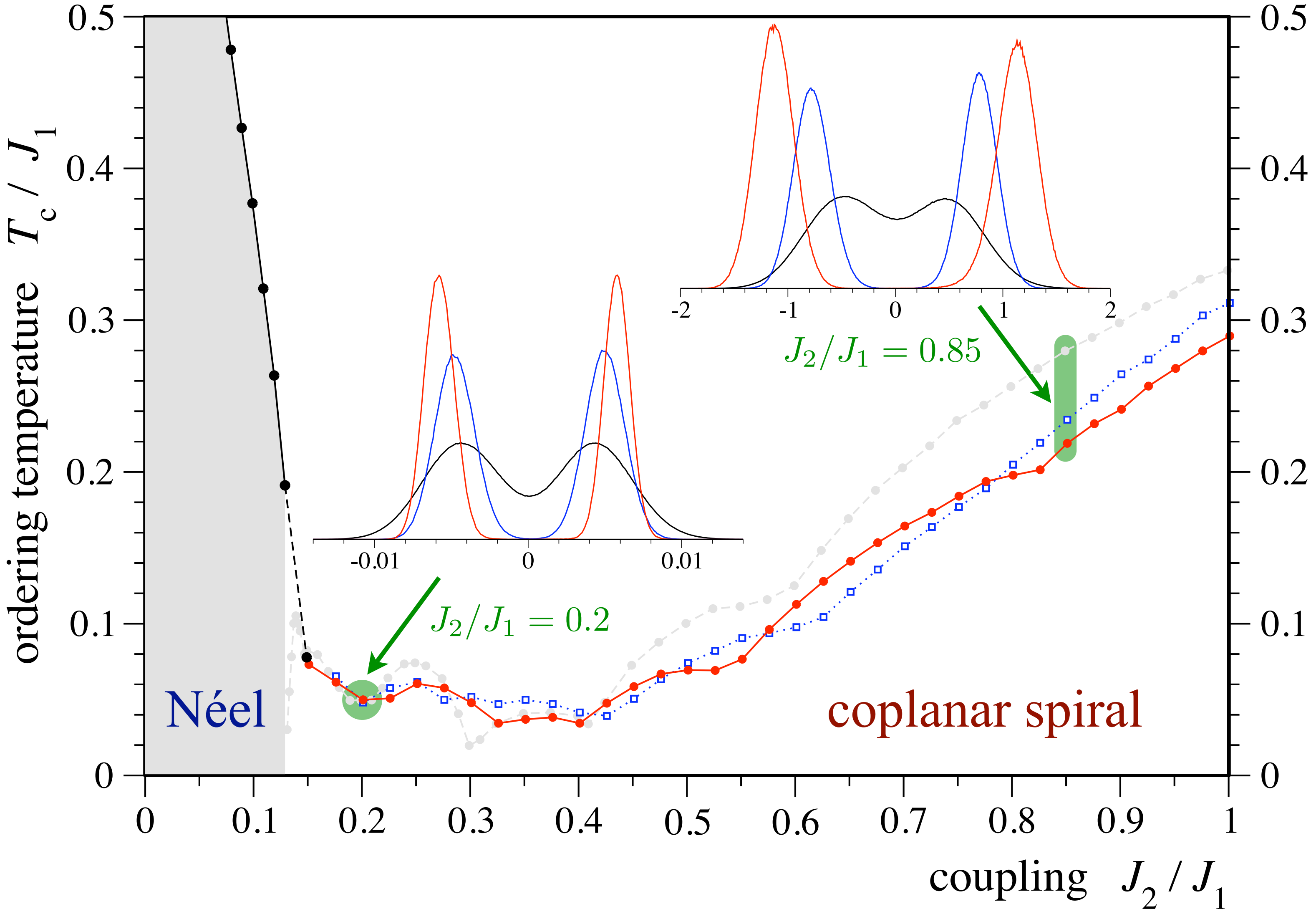
First-order transitions

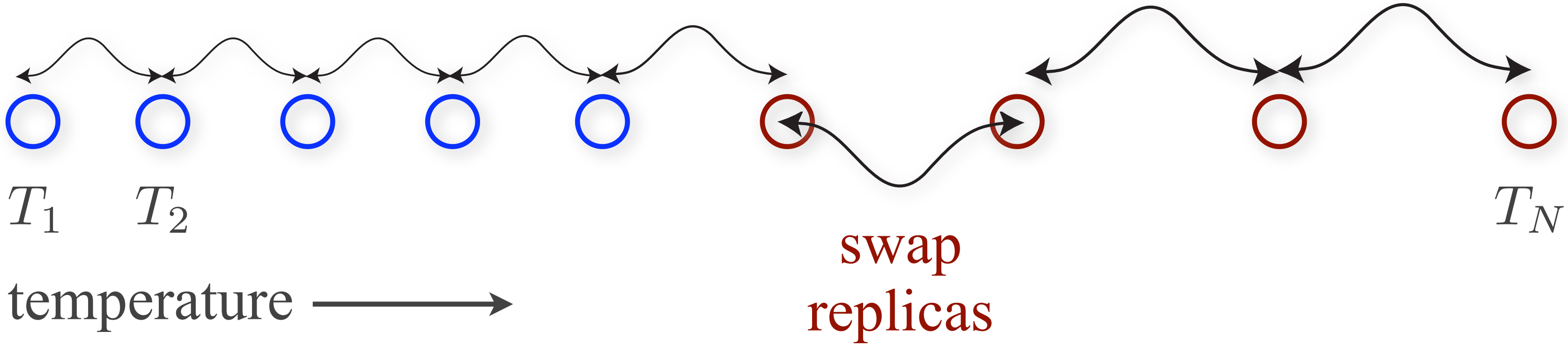




Parallel tempering

K. Hukushima and Y. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996)

Simulate **multiple replicas** of the system at various temperatures.



$$p(E_i, T_i \to E_{i+1}, T_{i+1}) = \min(1, \exp(\Delta\beta\Delta E))$$

Single replica performs **random walk** in temperature space.

How do we choose the temperature points?

Ensemble optimization

Feedback algorithm

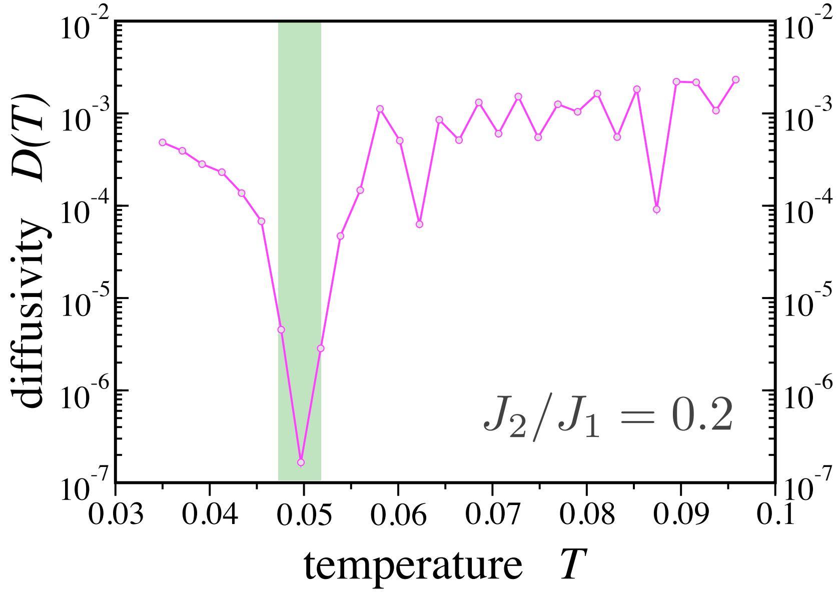
Measure **local diffusivity** $D(T)$ of current in temperature space.

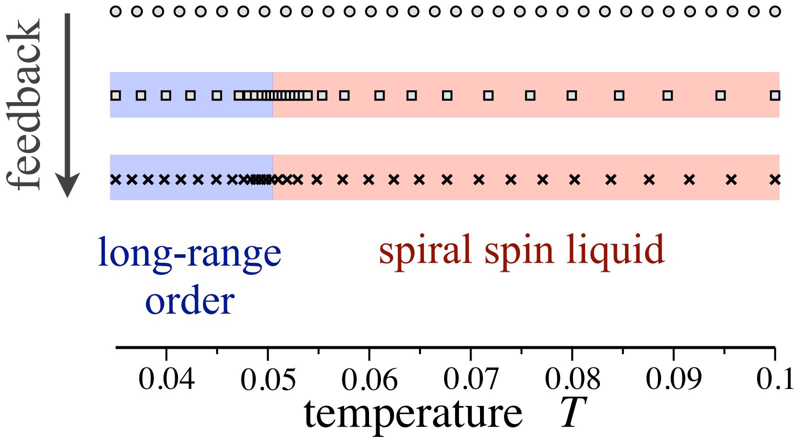
Optimal choice of temperatures

$$\boxed{\eta^{\text{opt}}(T)} \sim \frac{1}{\sqrt{D(T)}}$$

density of T-points

Iterate feedback of diffusivity.

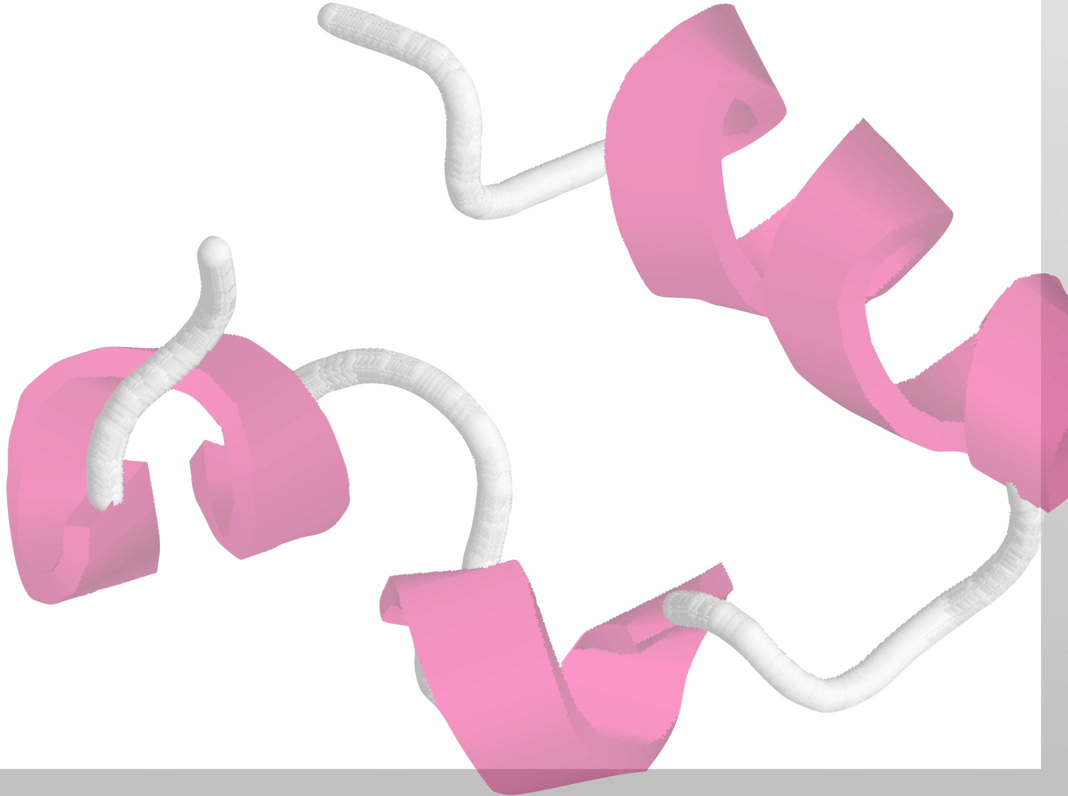




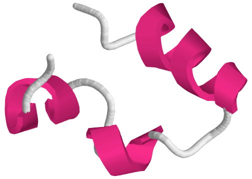
Example

Folding of a (small) protein

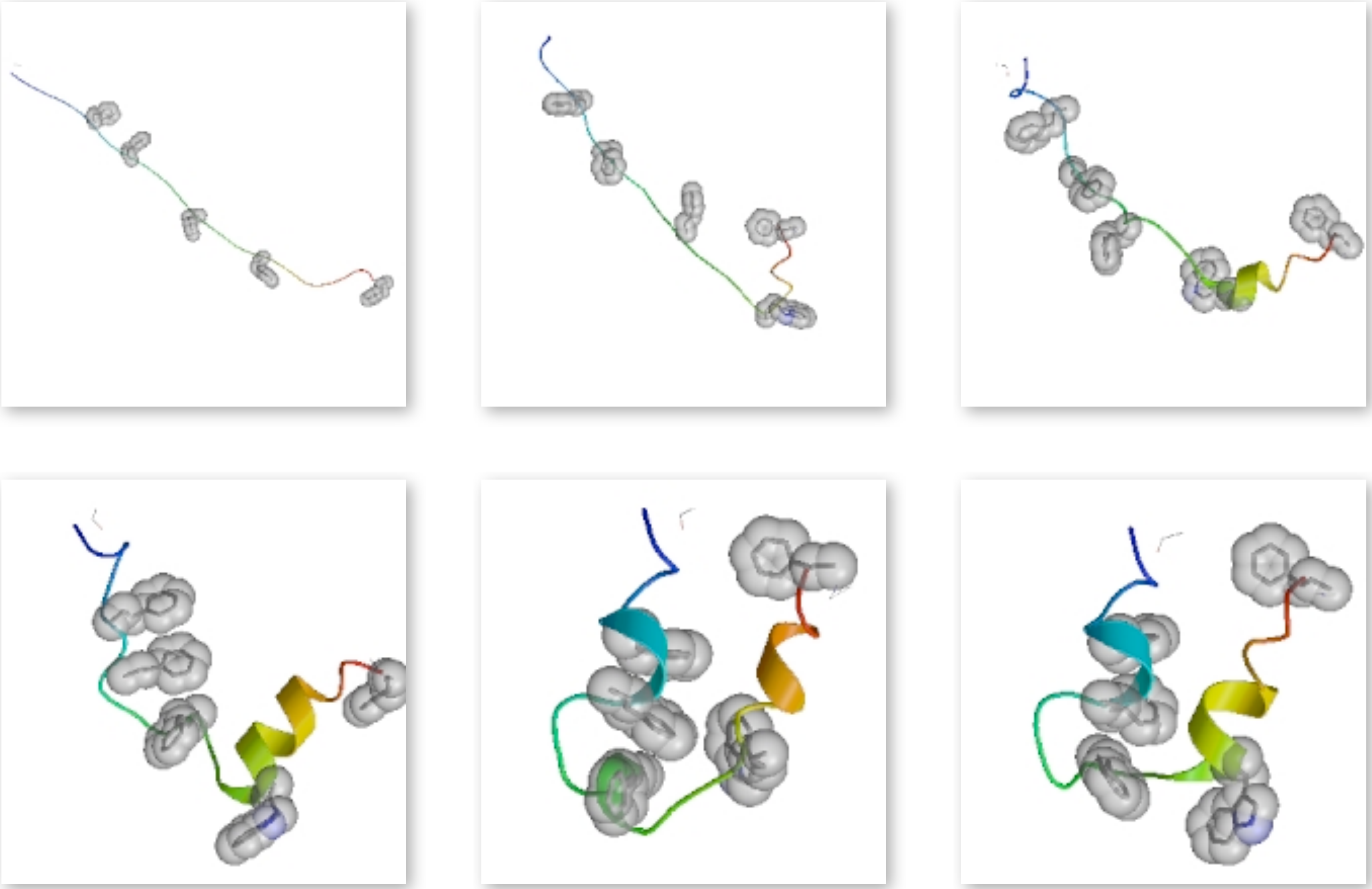
ST, M. Troyer, U.H.E. Hansmann
J. Chem. Phys. **124**, 174903 (2006).



A small protein: HP-36



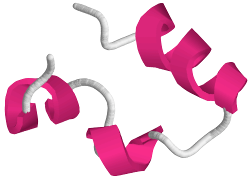
The chicken villin headpiece

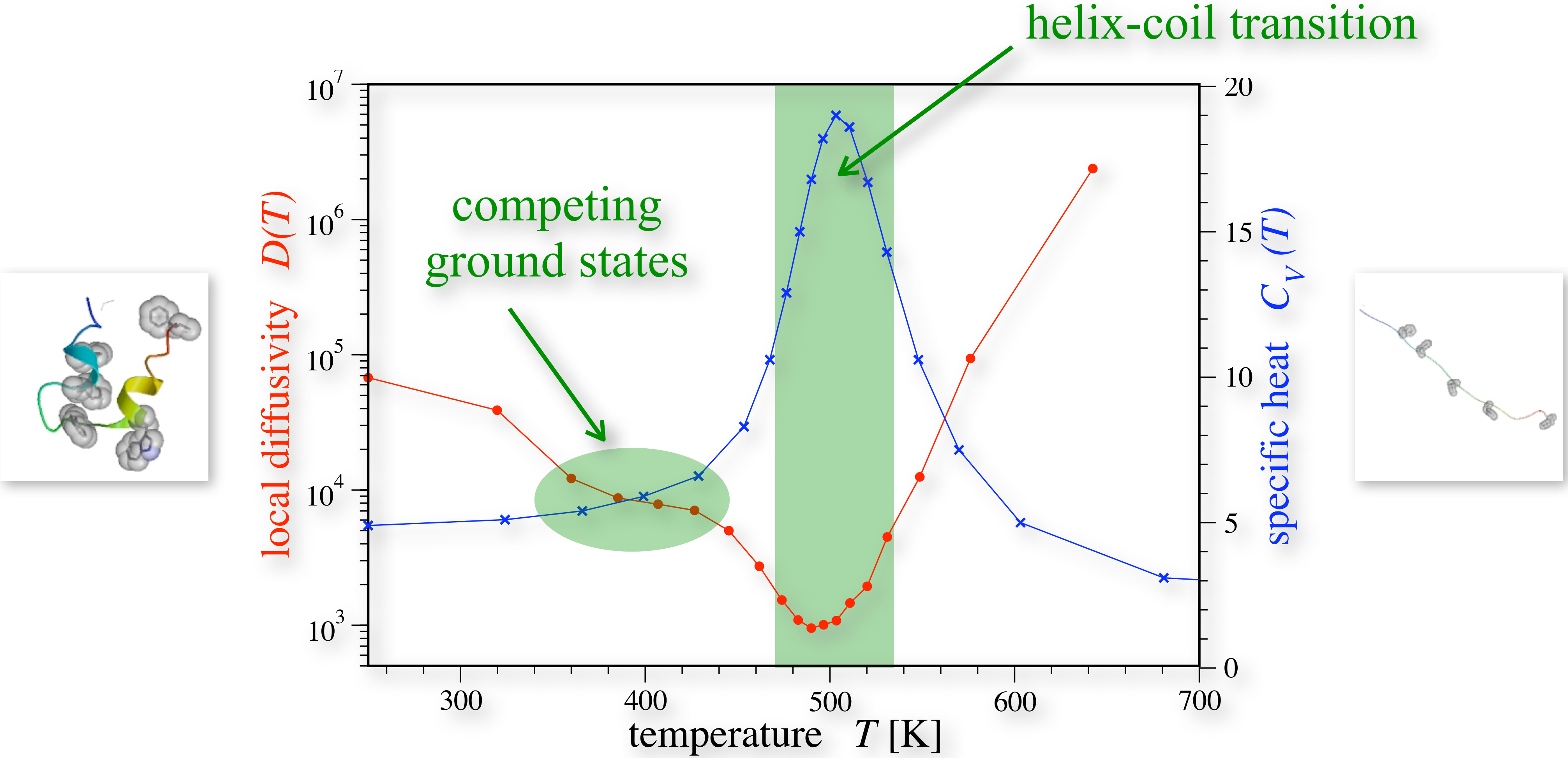


folding@home project

folding time: 4.3 microseconds

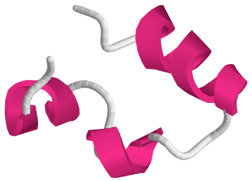
Random walk in temperature

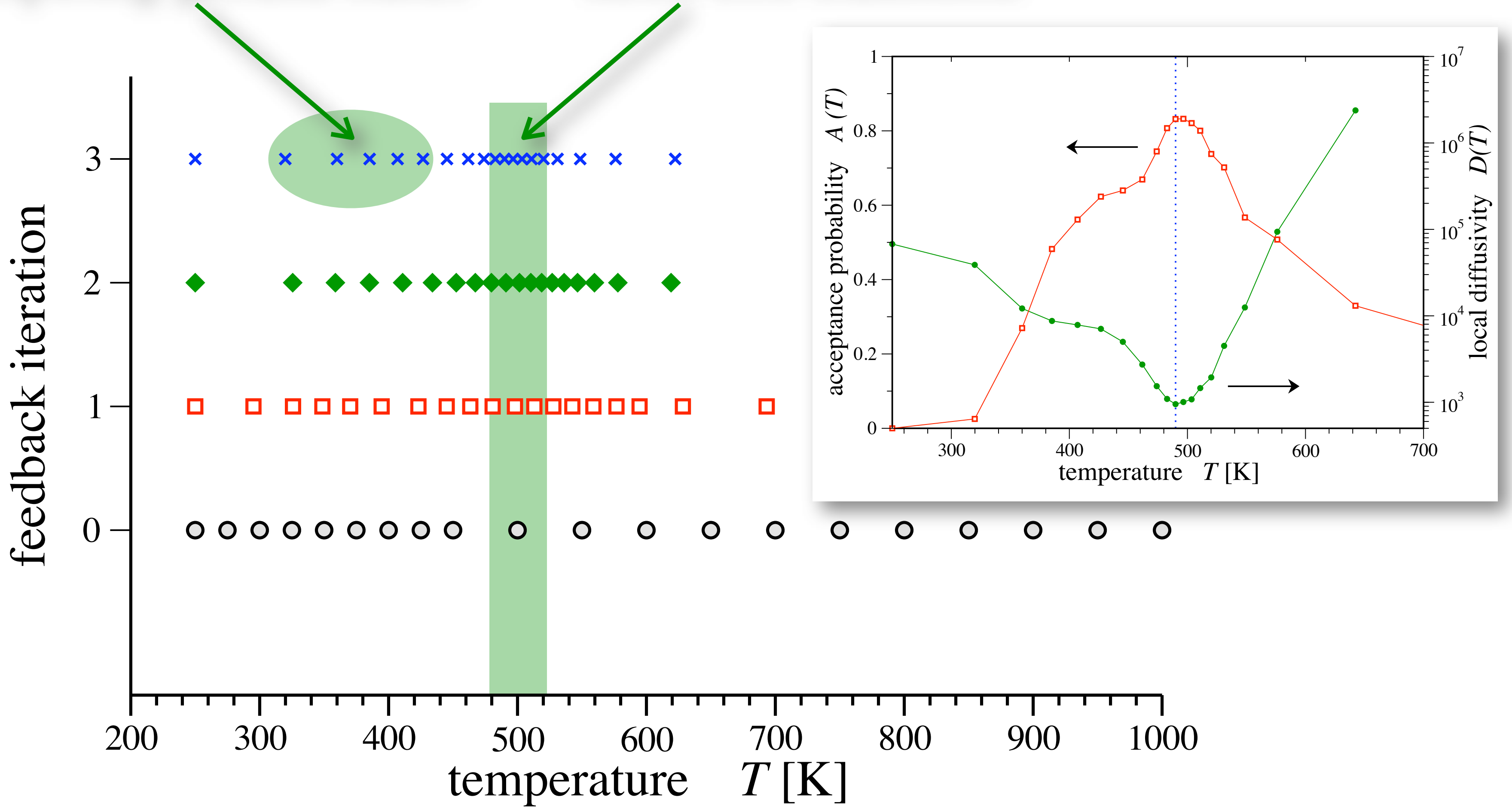




- **Multiple temperature scales** are revealed by the local diffusivity.

Optimized temperature sets





competing ground states

helix-coil transition

- Feedback reallocates resources towards the relevant temperature scales.

Example

Quantum systems

S. Wessel, N. Stoop, E. Gull, ST, M. Troyer
J. Stat. Mech. P12005 (2007).

$\hbar$

Quantum systems

$\hbar$

Reconsider the high-temperature series expansion

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}\, (-H)^n = \sum_{n=0}^{\infty} \boxed{g(n)}\, \beta^n$$

coefficients
"density of states"

We can define a broad-histogram ensemble in the expansion order.

M. Troyer, S. Wessel & F. Alet, PRL **90**, 120201 (2003).

Stochastic series expansion (SSE) samples these coefficients

$n \to 0$

high temperatures

?

$n \to \infty$

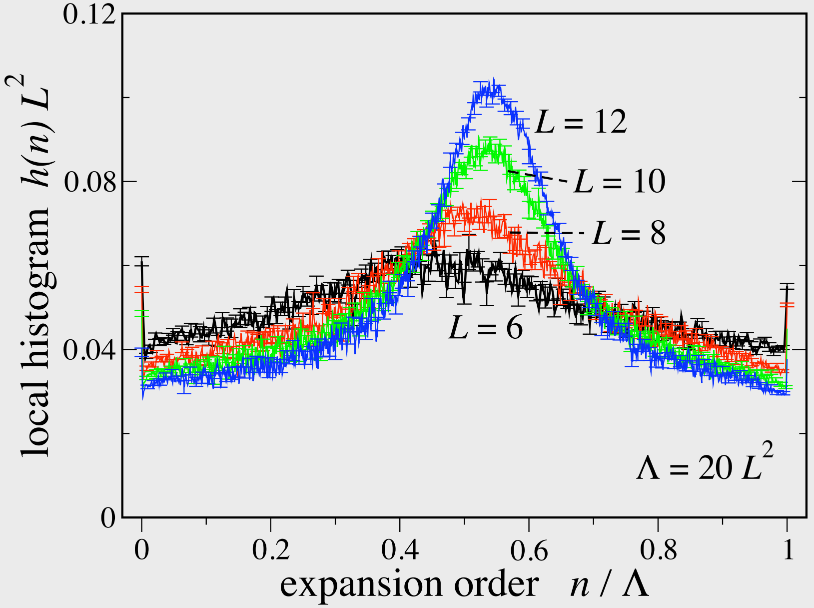
low temperatures

Examples

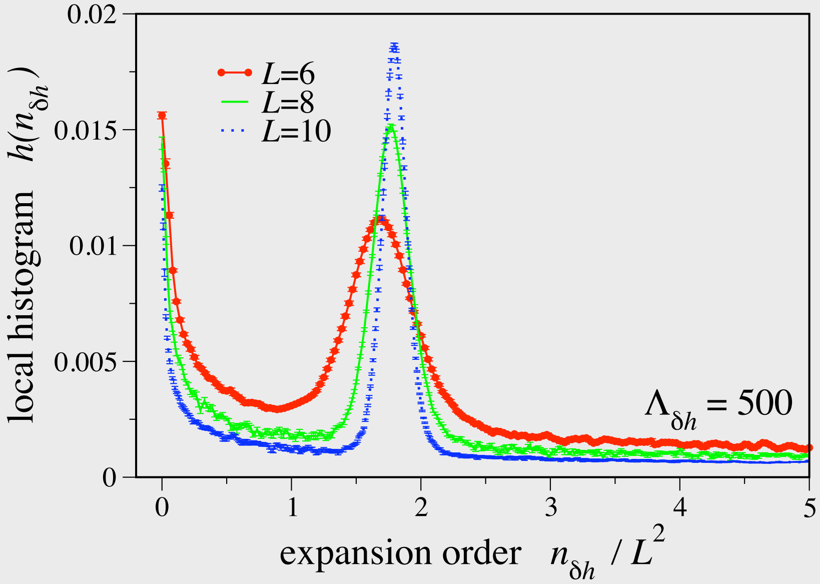
Thermal first-order transition

hard-core bosons
with next-nearest neighbor repulsion

$$H = -t \sum_{\langle i,j\rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V_2 \sum_{\langle\langle i,k\rangle\rangle} n_i n_k - \mu \sum_i n_i$$



Spin-flop transition



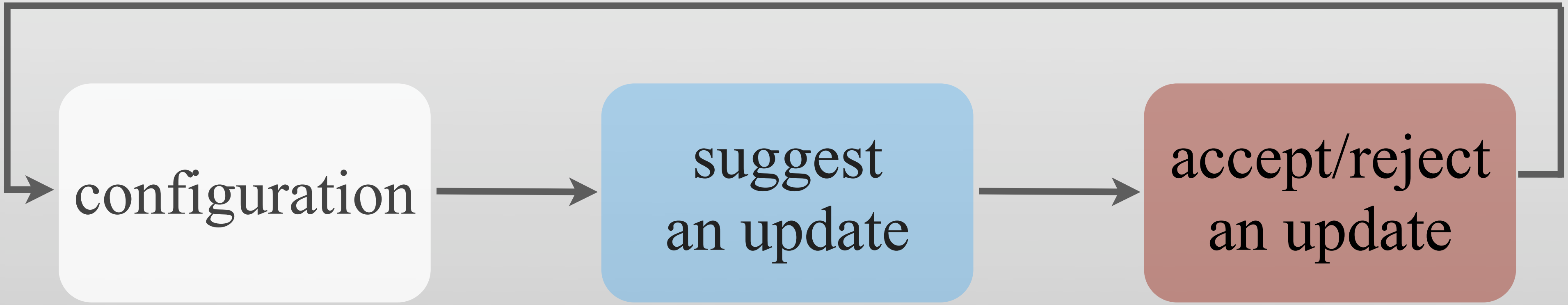
spin-1/2 XXZ model in a magnetic field

$$H = J \sum_{<i,j>} \left[S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z \right]$$

$$-h \sum_i S_i^z$$

Summary

Metropolis cycle



configuration

suggest an update

accept/reject an update

non-local update schemes
loops, worms, ...

unconventional
statistical ensembles